Ethyl orthoformate 122-51-0 | DTXSID8041957

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 21.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.94e-01

Confidence level: 5.85e-01

Nearest Neighbors from the Training Set

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Urea, (3-methylphenyl)-

Measured: 36.3 Predicted: 37.2

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N-Methyl-N'-phenylurea

Measured: 19.5 Predicted: 29.8

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Ethyl valerate Measured: 93.3 Predicted: 68.6

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1-Methoxy-2-propyl acetate

Measured: 2.29 Predicted: 7.33 Image not found

1-Phenylurea Measured: 22.4 Predicted: 34.2